

## METAL-ORGANIC COMPOUNDS

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**Organometallic Selenolates. VII. (Benzylselenolato-Se)tricarbonyl( $\eta^5$ -cyclopentadienyl)molybdenum(II) and Bis[1,2( $\eta^5$ -cyclopentadienyl)]-di- $\mu$ -ethylselenolato-di- $\mu$ -selenido-dimolybdenum(IV)(Mo—Mo)†**

CARSTEN THÖNE, PETER G. JONES AND JÖRG LAUBE

*Institut für Analytische und Anorganische Chemie, Technische Universität Braunschweig, Postfach 3329, 38023 Braunschweig, Germany. E-mail: thoene@xray36.anchem.nat.tu-bs.de*

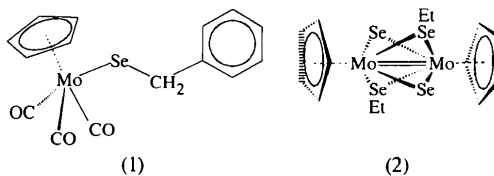
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**Abstract**

Compound (1),  $[\text{Mo}(\eta^5\text{-C}_5\text{H}_5)(\text{C}_7\text{H}_7\text{Se})(\text{CO})_3]$ , is monomeric in the solid state. The  $\text{Cp}(\text{CO})_3\text{MoSe}$  moiety (where Cp is cyclopentadienyl) displays a ‘piano-stool’ arrangement with an Mo—Se bond length of 2.6294 (4) Å and an essentially ideal tetrahedral bond angle at selenium [109.74 (8)°]. The binuclear compound (2),  $[\text{Mo}_2(\eta^5\text{-C}_5\text{H}_5)_2(\text{C}_2\text{H}_5\text{Se})_2(\text{Se})_2]$ , consists of linear Cp—Mo—Mo—Cp moieties with Mo=Mo double bonds, which are quadruply bridged by two pairs of selenido and ethylselenolato ligands.

**Comment**

Organoselenolato and selenido complexes of transition metals represent a growing field of current interest in structural chemistry because of the variety of features that can be observed in this class of compounds. Recently, we started an investigation of new synthetic routes to organoselenolato complexes (Eikens, Kienitz, Jones & Thöne, 1994; Eikens, Jäger, Jones & Thöne, 1996; Jones & Thöne, 1996; Eikens, Jäger, Jones, Laube & Thöne, 1996; Jones, Laube & Thöne, 1997; Eikens, Jones & Thöne, 1997) and present here the crystal structures of the two organoselenolato molybdenum complexes  $[\text{Mo}(\text{CO})_3(\eta^5\text{-C}_5\text{H}_5)(\text{C}_7\text{H}_7\text{Se})]$ , (1), and  $[\text{Mo}_2(\eta^5\text{-C}_5\text{H}_5)_2(\mu\text{-C}_2\text{H}_5\text{Se})_2(\mu\text{-Se})_2]$ , (2).



† Part VI: Eikens, Jones & Thöne (1997).

Compound (1) crystallizes in the monoclinic space group  $P2_1/c$  with one formula unit in the asymmetric unit. A comparison with the analogous tungsten complex (Eikens *et al.*, 1994) reveals that the structures are essentially isostructural without being isotopic. The unit cells display very similar axis lengths, although the tungsten analogue crystallizes with two independent formula units in the triclinic crystal system [ $\alpha = 91.99(3)$ ,  $\beta = 95.01(3)$  and  $\gamma = 90.08(3)^\circ$ ]; a search for higher metric symmetry offered monoclinic  $P$  as a possible choice ( $R_{\text{int}} = 0.2$ ), but the deviations from monoclinic symmetry, both metric and Laue, are too high. Nevertheless, the coordinates of (1) and one independent molecule of its tungsten analogue correspond closely to each other.

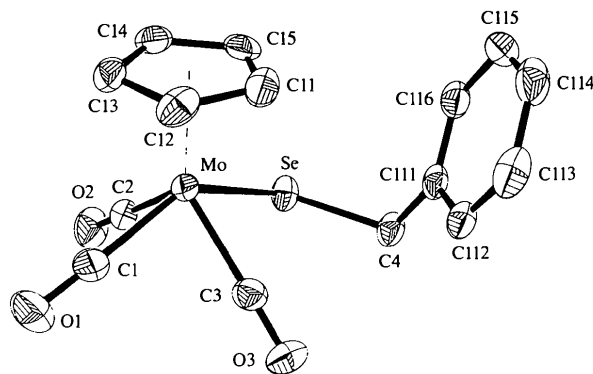


Fig. 1. The structure of molecule (1) in the crystal. Radii are arbitrary. H atoms have been omitted. Ellipsoids are drawn at the 50% probability level.

The  $\text{Cp}(\text{CO})_3\text{MoSe}$  moiety displays the commonly observed ‘piano-stool’ conformation with the corresponding angles 73.59 (7) (C2—Mo—Se), 76.02 (C3—Mo—Se), 77.49 (11) (C1—Mo—C2), 78.18 (10) (C1—Mo—C3), 101.63 (10) (C2—Mo—C3) and 135.96 (7)° (C1—Mo—Se), and an ideal tetrahedral angle at selenium [C4—Se—Mo 109.74 (8)°].

Consistent with the above discussion, bond lengths and angles in (1) display approximately the same values as in the tungsten derivative (Eikens *et al.*, 1994). The Mo—Se bond length [2.6294 (4) Å] indicates an Mo—Se single bond, comparable with the corresponding bonds in  $[(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_2\text{Mo}\{\mu\text{-SeCH}_2\text{C}(\text{CH}_3)=\text{CH}_2\}]_2$  [2.6327 (8) Å, average of four Mo—Se bonds; Jones *et al.*, 1997],  $(\text{NEt}_4)[(\eta^5\text{-C}_5\text{H}_5)\text{Mo}(\text{CO})_2\text{Se}_2]$  [2.598 (1) and 2.596 (1) Å; Adel, Weller & Dehnicke, 1988],  $[(\eta^5\text{-C}_5\text{Me}_5)\text{Mo}(\text{NO})(\mu\text{-Se}_2)]_2$  [2.566 (2), 2.634 (2) and 2.648 (2) Å; Herberhold, Jin & Rheingold, 1993] and  $[(\eta^7\text{-C}_7\text{H}_7)\text{Mo}(\mu\text{-SePh})_3\text{Mo}(\text{CO})_3]$  [2.563 (1), 2.565 (3) and 2.675 (2) Å;

Rettenmaier, Weidenhammer & Ziegler, 1981]. These values lie in the upper range of observed Mo—Se single bond lengths (2.4–2.7 Å), which are strongly influenced by steric and electronic effects and also by the bonding mode of the Se-containing ligands.

The crystal structure of compound (2) is shown in Fig. 2. The molecule, which possesses crystallographic inversion symmetry, consists of a linear Cp—Mo—Mo—Cp unit, with the  $\pi$ -bonded Cp ligands perpendicular to the Mo=Mo bond. Consistent with the 18 valence-electron rule and the short Mo—Mo bond length of 2.6399(6) Å, this value can be assigned as an Mo=Mo double bond (Endrich, Korswagen, Zahn & Ziegler, 1982) and is comparable with that in the analogous phenylselenolato compound  $[(\eta^5\text{-C}_5\text{H}_5)\text{Mo}(\mu\text{-Se})(\mu\text{-SePh})_2]$  [2.653(2) Å; Rakoczy, Schollenberger, Nuber & Ziegler, 1994].

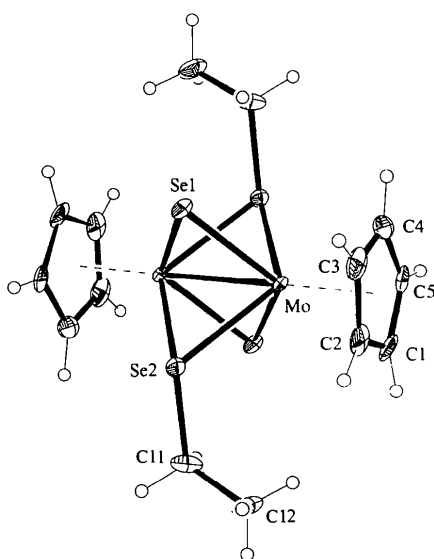


Fig. 2. The structure of molecule (2) in the crystal. Radii are arbitrary. Ellipsoids are drawn at the 50% probability level.

The Mo=Mo double bond is quadruply bridged by two alternate pairs of monoselenido and ethylselenolato ligands. The Mo atoms lie in an exact plane, with the Se1 and Se1<sup>i</sup> (selenido bridge) atoms on one side and Se2 and Se2<sup>i</sup> (ethylselenolato bridge) on the other side, with an interplanar angle of 85.44(2)°. Short contacts between the Se atoms are observed [Se1···Se2 2.941(1) and Se1···Se2<sup>i</sup> 3.185(1) Å; symmetry code: (i) 1 - x, 1 - y, -z].

The Mo—Se bond lengths differ greatly because of the different coordination numbers of selenium. In the case of the selenido bridge, the values are 2.4816(5) (Mo—Se1) and 2.4838(5) Å (Mo—Se1<sup>i</sup>). The corresponding Mo—SeEt bond lengths are 2.5902(6) (Mo—Se2) and 2.5943(5) Å (Mo—Se2<sup>i</sup>). The same bonding situation can be found in the phenyl-substituted derivative (Rakoczy *et al.*,

1994), which, however, has no crystallographic symmetry [Mo—( $\mu$ -Se) 2.460(2), 2.465(2), 2.503(2) and 2.507(2) Å; Mo—( $\mu$ -SePh) 2.583(2), 2.597(2), 2.607(2) and 2.612(2) Å]. Associated with additional electronic influences, smaller values for the Mo—Se (selenido bridge) bond lengths were observed in *trans*- $[(\eta^5\text{-C}_5\text{H}_5)\text{Mo}(\text{O})(\mu\text{-Se})_2(\text{Mo—Mo})]$  [2.452(1) and 2.448(1) Å], *cis*- $[(\eta^5\text{-C}_5\text{H}_5)\text{Mo}(\text{O})(\mu\text{-Se})_2(\text{Mo—Mo})]$  [2.428(1)–2.442(1) Å], *trans*- $[(\eta^5\text{-C}_5\text{H}_5)\text{Mo}(\text{O})(\mu\text{-Se})(\mu\text{-O})_2(\text{Mo—Mo})]$  [2.449(1) and 2.453(1) Å; Gorzelli, Bock, Gang, Nuber & Ziegler, 1991], *cis*- $[(\eta^5\text{-C}_5\text{Me}_5)\text{Mo}(\text{O})(\mu\text{-Se})_2(\text{Mo—Mo})]$  [2.422(2) and 2.431(2) Å; Endrich, Guggolz, Serhadle, Ziegler & Korswagen, 1988] and  $[(\eta^5\text{-C}_5\text{H}_4\text{Pr})\text{Mo}(\mu_3\text{-Se})_4(\text{Mo—Mo})]$  (2.464 Å, no s.u. given; Baird *et al.*, 1991). The ethylselenolato Se atoms display almost tetrahedral bond angles [C11—Se2—Mo 113.11(10) and C11—Se2—Mo<sup>i</sup> 112.92(9)°], whereas the angles belonging to the Mo<sub>2</sub>Se<sub>4</sub> core are acute [Mo—Se—Mo<sup>i</sup> 64.234(13) and Mo—Se2—Mo<sup>i</sup> 61.219(12)°]. The accompanying angles at the Mo atoms are comparable (see Table 2).

## Experimental

Compound (1) was obtained as the main product from the reaction of LiSeMo(CO)<sub>3</sub>( $\eta^5\text{-C}_5\text{H}_5$ ) with C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>Cl according to Eikens *et al.* (1994). Single crystals were obtained by cooling a saturated ethanol solution to 253 K. Compound (2) was obtained as a by-product from the reaction of LiSeSeMo(CO)<sub>3</sub>( $\eta^5\text{-C}_5\text{H}_5$ ) with C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>Cl in the presence of LiBEt<sub>3</sub>H as reducing agent. Single crystals were obtained by layering a dichloromethane solution with hexanes.

## Compound (1)

### Crystal data

[Mo(C<sub>5</sub>H<sub>5</sub>)(C<sub>7</sub>H<sub>7</sub>Se)(CO)<sub>3</sub>]

$M_r = 415.15$

Monoclinic

$P2_1/c$

$a = 9.8918(10)$  Å

$b = 11.6789(12)$  Å

$c = 12.6536(12)$  Å

$\beta = 95.819(8)^\circ$

$V = 1454.3(3)$  Å<sup>3</sup>

$Z = 4$

$D_x = 1.896$  Mg m<sup>-3</sup>

$D_m$  not measured

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 62 reflections

$\theta = 5.5\text{--}12.5^\circ$

$\mu = 3.407$  mm<sup>-1</sup>

$T = 173(2)$  K

Tablet

$0.40 \times 0.36 \times 0.22$  mm

Red

### Data collection

Siemens P4 diffractometer

$\omega$  scans

Absorption correction:

$\psi$  scans (XEMP in XSCANS; Siemens, 1994b)

$T_{\min} = 0.31$ ,  $T_{\max} = 0.47$

3851 measured reflections

2553 independent reflections

2177 reflections with

$I > 2\sigma(I)$

$R_{\text{int}} = 0.021$

$\theta_{\max} = 24.99^\circ$

$h = 0 \rightarrow 11$

$k = -13 \rightarrow 5$

$l = -14 \rightarrow 14$

3 standard reflections

every 247 reflections

intensity decay: 2%

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.019$   
 $wR(F^2) = 0.042$   
 $S = 0.976$   
 2553 reflections  
 182 parameters  
 H-atom parameters  
 constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0205P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = -0.001$   
 $\Delta\rho_{\max} = 0.265 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.325 \text{ e } \text{Å}^{-3}$   
 Extinction correction:  
*SHELXL93*  
 Extinction coefficient:  
 0.0019 (2)  
 Scattering factors from  
*International Tables for*  
*Crystallography* (Vol. C)

Table 1. Selected geometric parameters ( $\text{Å}$ ,  $^\circ$ ) for (1)

Mo—C1	1.992 (3)	C1—O1	1.140 (3)
Mo—C3	1.995 (3)	C2—O2	1.141 (3)
Mo—C2	1.996 (3)	C3—O3	1.140 (3)
Mo...Cp(centre)	2.014	Se—C4	1.981 (2)
Mo—Se	2.6294 (4)	C4—C111	1.498 (3)
C1—Mo—C3	78.18 (10)	O1—C1—Mo	179.0 (2)
C1—Mo—C2	77.49 (11)	O2—C2—Mo	178.9 (2)
C3—Mo—C2	101.63 (10)	O3—C3—Mo	178.6 (2)
C1—Mo—Se	135.96 (7)	C4—Se—Mo	109.74 (8)
C3—Mo—Se	76.02 (7)	C111—C4—Se	115.09 (17)
C2—Mo—Se	73.59 (7)		

## Compound (2)

## Crystal data

$[\text{Mo}_2(\text{C}_5\text{H}_5)_2(\text{C}_2\text{H}_5\text{Se})_2(\text{Se})_2]$   
 $M_r = 696.02$   
 Monoclinic  
 $P2_1/c$   
 $a = 8.4036 (15) \text{ Å}$   
 $b = 15.376 (3) \text{ Å}$   
 $c = 6.9712 (12) \text{ Å}$   
 $\beta = 99.092 (8)^\circ$   
 $V = 889.5 (3) \text{ Å}^3$   
 $Z = 2$   
 $D_x = 2.599 \text{ Mg m}^{-3}$   
 $D_m$  not measured

Mo  $K\alpha$  radiation  
 $\lambda = 0.71073 \text{ Å}$   
 Cell parameters from 62  
 reflections  
 $\theta = 5.0\text{--}12.5^\circ$   
 $\mu = 9.582 \text{ mm}^{-1}$   
 $T = 173 (2) \text{ K}$   
 Prism  
 $0.30 \times 0.16 \times 0.12 \text{ mm}$   
 Red

## Data collection

Siemens P4 diffractometer  
 $\omega$  scans  
 Absorption correction:  
 $\psi$  scans (*XEMP* in  
*XSCANS*; Siemens, 1994b)  
 $T_{\min} = 0.127$ ,  $T_{\max} = 0.317$   
 3101 measured reflections  
 1555 independent reflections  
 1497 reflections with  
 $I > 2\sigma(I)$

$R_{\text{int}} = 0.041$   
 $\theta_{\max} = 24.99^\circ$   
 $h = -9 \rightarrow 9$   
 $k = -18 \rightarrow 0$   
 $l = -8 \rightarrow 8$   
 3 standard reflections  
 every 247 reflections  
 intensity decay: 1%

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.019$   
 $wR(F^2) = 0.047$   
 $S = 1.093$   
 1554 reflections  
 93 parameters  
 H-atom parameters  
 constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0202P)^2 + 0.1393P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.587 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.619 \text{ e } \text{Å}^{-3}$   
 Extinction correction:  
*SHELXL93*  
 Extinction coefficient:  
 0.0146 (6)  
 Scattering factors from  
*International Tables for*  
*Crystallography* (Vol. C)

Table 2. Selected geometric parameters ( $\text{Å}$ ,  $^\circ$ ) for (2)

Mo...Cp(centre)	2.001	Mo—Mo'	2.6399 (6)
Mo—Se1	2.4816 (5)	Se2—C11	1.979 (3)
Mo—Se1'	2.4838 (5)	C11—C12	1.511 (5)
Mo—Se2	2.5902 (6)	Se1—Se2	2.941 (1)
Mo—Se2'	2.5943 (5)	Se1—Se2'	3.185 (1)
Se1—Mo—Se1'	115.766 (13)	Mo—Se1—Mo'	64.234 (13)
Se1—Mo—Se2	70.860 (11)	C11—Se2—Mo	113.11 (10)
Se1'—Mo—Se2	77.740 (15)	C11—Se2—Mo'	112.92 (9)
Se1—Mo—Se2'	77.70 (2)	Mo—Se2—Mo'	61.219 (12)
Se1'—Mo—Se2'	70.76 (2)	C12—C11—Se2	111.1 (2)
Se2—Mo—Se2'	118.781 (12)		

Symmetry code: (i)  $1 - x, 1 - y, -z$ .

H atoms were included using rigid methyl groups (allowed to rotate but not tip) or a riding model.

For both compounds, data collection: *XSCANS* (Siemens, 1994b); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structures: *SHELXS86* (Sheldrick, 1990); program(s) used to refine structures: *SHELXL93* (Sheldrick, 1993); molecular graphics: *XP* (Siemens, 1994a); software used to prepare material for publication: *SHELXL93*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FG1338). Services for accessing these data are described at the back of the journal.

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**Oxo-1κO-μ<sub>3</sub>-(pyridine-2-thiolato-2κN,-3:4κ<sup>2</sup>S)-tri-μ<sub>3</sub>-sulfido-1:2:3κ<sup>3</sup>S;1:2:4κ<sup>3</sup>S;-2:3:4κ<sup>3</sup>S-tris(triphenylphosphine)-2κP;-3κP;4κP-tricoppermolybdenum**

QUANMING WANG, XINTAO WU,\* QUN HUANG, TIANLU SHENG AND PING LIN

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China. E-mail: wxt@ms.fjirsm.ac.cn

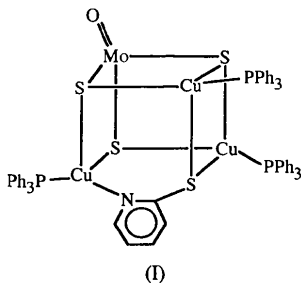
(Received 6 November 1996; accepted 6 March 1997)

**Abstract**

The title compound, [MoO{μ<sub>3</sub>-Cu(C<sub>18</sub>H<sub>15</sub>P)}<sub>3</sub>(μ<sub>3</sub>-S)<sub>3</sub>-(μ<sub>3</sub>-C<sub>5</sub>H<sub>4</sub>NS)], contains an incomplete cubane-like cluster core, [MoCu<sub>3</sub>S<sub>3</sub>(C<sub>5</sub>H<sub>4</sub>NS)]<sup>2+</sup>, in which the S and N atoms of a pyridine-2-thiolato ligand bridge three Cu atoms.

**Comment**

Recently, some incomplete cubane-like heterometallic clusters belonging to the M/Cu/S (M = Mo or W) system have been synthesized in our laboratory. For example, clusters containing the cores [M<sub>2</sub>CuS<sub>4</sub>]<sup>3+</sup> (Zhu, Zheng & Wu, 1990), [MoCu<sub>3</sub>S<sub>3</sub>(S<sub>2</sub>COEt)]<sup>2+</sup> (Zhu, Du, Chen & Wu, 1992) and [WCu<sub>3</sub>S<sub>3</sub>{S<sub>2</sub>P(COEt)<sub>2</sub>}]<sup>2+</sup> (Du & Wu, 1994) have been prepared. The structure of the title compound, (I), is similar to that of [MoCu<sub>3</sub>S<sub>3</sub>-(S<sub>2</sub>COEt)(O)(PPh<sub>3</sub>)<sub>3</sub>], except that S<sub>2</sub>COEt<sup>-</sup> is replaced by a bidentate pyridine-2-thiolato ligand.



(I)

As shown in Fig. 1, the Mo atom in (I) has tetrahedral coordination, MoOS<sub>3</sub><sup>2-</sup>; furthermore, each Cu atom is coordinated by a distorted tetrahedron of

two S atoms of tetradentate MoOS<sub>3</sub><sup>2-</sup>, one P atom of PPh<sub>3</sub> and one S (or N) atom of the pyridine-2-thiolato ligand. The average Mo···Cu, μ<sub>3</sub>-S—Mo and μ<sub>3</sub>-S—Cu distances of 2.738 (2), 2.255 (3) and 2.310 (3) Å, respectively, are comparable with the corresponding values of 2.735 (1), 2.255 (2) and 2.302 (2) Å found in [MoCu<sub>3</sub>S<sub>3</sub>(S<sub>2</sub>COEt)(O)(PPh<sub>3</sub>)<sub>3</sub>]. The mean Cu—S bond length (of C<sub>5</sub>H<sub>4</sub>NS<sup>-</sup>) is 2.458(3) Å and the Cu—N bond length is 2.103 (9) Å.

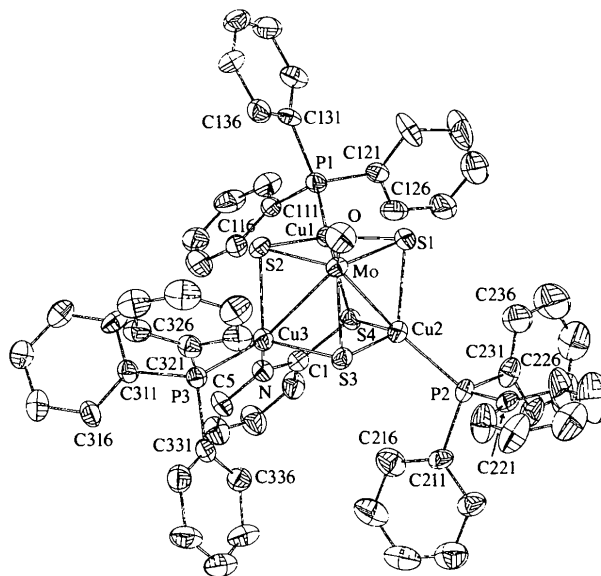


Fig. 1. The molecular structure of (I) showing 40% probability displacement ellipsoids. For clarity, H atoms have been omitted. The phenyl C atoms are numbered sequentially around each ring.

**Experimental**

The title compound was synthesized by reaction of [MoCu<sub>2</sub>S<sub>3</sub>](O)(PPh<sub>3</sub>)<sub>3</sub> with C<sub>5</sub>H<sub>4</sub>NSCu in CH<sub>2</sub>Cl<sub>2</sub>. Black crystals were obtained by evaporating the filtrate for several days after addition of 2-propanol.

*Crystal data*

[Cu<sub>3</sub>Mo(O)S<sub>3</sub>(C<sub>5</sub>H<sub>4</sub>NS)-(C<sub>18</sub>H<sub>15</sub>P)<sub>3</sub>]

*M<sub>r</sub>* = 1295.79

Triclinic

*P*1

*a* = 10.131 (3) Å

*b* = 12.711 (5) Å

*c* = 23.594 (7) Å

α = 87.27 (3)°

β = 101.59 (3)°

γ = 109.05 (3)°

*V* = 2813 (2) Å<sup>3</sup>

*Z* = 2

*D<sub>x</sub>* = 1.53 Mg m<sup>-3</sup>

*D<sub>m</sub>* not measured

Mo Kα radiation

λ = 0.71073 Å

Cell parameters from 19 reflections

θ = 9–11°

μ = 1.60 mm<sup>-1</sup>

*T* = 293 K

Rectangular

0.22 × 0.20 × 0.12 mm

Black